

Gaussian Overlap Approximation for the quadrupole collective states

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Abstract. The Generator Coordinate Method (GCM) in the Gaussian Overlap Approximation (GOA) is applied to a description of the nuclear quadrupole collective states. The full five-dimensional quadrupole tensor is used as a set of the generator coordinates. The integral Hill-Wheeler equation is reduced to a differential equation by using the Fourier transforms of the overlap and energy kernels. The differential Bohr Hamiltonian obtained this way is compared with that derived by the usual approach to the collective Hamiltonian in the GOA which does contain an additional approximation. The method of calculating the quantities which determine the Bohr Hamiltonian from the set of deformation-dependent intrinsic states is demonstrated. In particular, it appears that the moments of inertia at the quadrupole rotations are of the type of that of Yoccoz.

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1. Introduction

The Bohr Hamiltonian (cf a recent review [1]) still remains one of the most effective tools to describe the lowest collective quadrupole excitations of the even-even nuclei. This is in spite of a long history of the collective model dated from the fifties of the twentieth century [2]. The rudiments of the model can be met even earlier [3]. Nowadays the Bohr Hamiltonian in a general form proposed in [4, 5] is considered. It is based on the correspondence principle, that is, on the assumption that the collective quadrupole motion has its classical counterpart. The quantum Bohr Hamiltonian is constructed from the most general classical Hamiltonian quadratic in velocities by the Podolsky-Pauli quantization prescription [6, 7, 8]. The quantum kinetic energy operator is then the Laplace-Beltrami operator in the Riemannian space with the metric tensor equal to the classical inertial matrix. Derivations of the Bohr Hamiltonian from the microscopic many-body theories of nuclei used so far, which are based on methods of the type of the Time-Dependent Hartree-Fock method, do pass through their classical stage too. The collective motion is then represented by a wave packet, which keeps the classical law of motion, requantized afterwards (cf e.g. [9, 1]).

A possibility of a purely quantum description of collective excitations is created by the Generator Coordinate Method (GCM) [10, 11] (see also [12]). The method leads originally to an integral eigenvalue equation (the Hill-Wheeler equation). The integral equation can be approximated by a differential equation of the Schrödinger type [13]. It is especially easy to do when the Gaussian Overlap Approximation (GOA) is made for overlap and energy kernels in the Hill-Wheeler equation [11, 14, 15]. The method is usually demonstrated for a single generator coordinate. But the quadrupole motion has five degrees of freedom and thus five generator coordinates are required. The multi-dimensional GCM was already considered by several authors [16, 17, 18, 19] (see also the review article [20]). Obviously, the GCM, being one of the contemporary tools for investigations of various collective phenomena and for the restoration of broken symmetries, has been applied to various problems in the nuclear physics apart from the quadrupole collective motion. The two-dimensional Hill-Wheeler equation has been used to investigate the quadrupole β and γ vibrations [21, 22, 23]. Before that the differential equations coming from the GOA have been applied to these vibrations [24, 25, 26, 27]. The GOA has been used to estimate the ground-state correlations associated with the quadrupole collective modes [28]. But the rotational correction to the ground-state energy has been obtained through the projection onto the good-angular-momentum state. The five-dimensional collective quadrupole Hamiltonian based on the GOA has been generated from the microscopic theory with the Gogny effective forces and used in comprehensive calculations of the 2^+ nuclear excitations [29]. However, the moments of inertia obtained by the Thouless-Valatin prescription [30] instead of those derived from the GOA are used in the Bohr Hamiltonian. In spite of these developments, it seems there is no consistent derivation of the full five-dimensional Bohr Hamiltonian using the GCM with the GOA yet.

The present study is devoted to application of the multi-dimensional GCM in the GOA to the five-dimensional quadrupole collective motion of the even-even nuclei. The quadrupole deformation tensor plays a role of a set of the five generator coordinates. We aim at deriving the Bohr Hamiltonian in a purely quantum way. The Hamiltonian obtained in such a way is a bit more general than that based on the correspondence principle (cf [1]). In order to transform the Hill-Wheeler integral eigenvalue equation into the Schrödinger differential equation with the Bohr Hamiltonian we introduce, after Onishi and Une [17], new quadrupole variables which diagonalise the exponent of the Gaussian overlap. Using these new variables we perform the Fourier analysis of the energy kernel. The kernel turns out to be a local distribution containing the Dirac delta function and its derivatives of the second order. It allows us to reduce the integral equation to a differential one. The Hamiltonian of the rigid rotor was derived earlier using the same method [31]. We compare the method of the Fourier analysis with the method used usually in deriving the collective Hamiltonian from the GCM [12, 20, 19]. The latter method contains an additional approximation apart from the GOA.

We formulate the Hill-Wheeler theory for the quadrupole collective excitations in section 2. Section 3 is devoted to the Gaussian Overlap Approximation for the quadrupole generator coordinates. The differential equation equivalent to the Hill-Wheeler equation in the GOA is derived and compared with the usual collective approach to the GCM in section 4.1. Formulae for calculating the quantities determining the overlaps within the GOA and the Bohr Hamiltonian from the deformation-dependent intrinsic state are given in section 5. We draw conclusions from the present study in section 6. In Appendix A the semi-Cartesian Wigner functions are introduced, which are convenient to use in the present study. The structure of matrices being isotropic functions of the quadrupole variables is discussed in Appendix B.

2. The Hill-Wheeler theory of the quadrupole collective excitations

2.1. The quadrupole generating states

Let the considered nucleus with Z protons and N neutrons be described microscopically by the many-body Hamiltonian \hat{H} which is invariant under the $O^T(3)$ group of transformations i.e. the superposition of time reversal \hat{T} and the orthogonal transformations (the rotations $\hat{R}(\omega)$ and the space inversion \hat{P}) in the physical three-dimensional space. In order to describe its quadrupole collective excitations by means of the GCM we start with states parametrised by the two deformation parameters d_0 and d_2 which describe the quadrupole deformation with respect to a system of principal axes. For instance, the intrinsic components of the mass quadrupole moment in the deformed ground state can serve as such parameters. Parameters d_0 and d_2 define the deformation (e.g., a shape) up to the group of five permutations of the principal axes (cf [1]). One of the principal axes is the symmetry axis when one of the three following conditions for the deformation parameters is fulfilled: $d_2 = 0$, $d_2 = \pm\sqrt{3}d_0$. The conditions represent

the three straight lines (or the six rays) intersecting each other at point $d_0 = 0$, $d_2 = 0$ on plane (d_0, d_2) of the deformation parameters. The rays divide the plane into the six sectors. The values of d_0 and d_2 located in one of the sectors describe the all possible deformations (shapes) at the established names of principal axes. The standard choice of the sector is the following:

$$0 \leq d_2 \leq \sqrt{3}d_0 < +\infty, \quad (2.1)$$

which means that the symmetry axes are z and y for $d_2 = 0$ and $d_2 = \sqrt{3}d_0$, respectively. Here, we assume that the ranges of values of d_0 and d_2 are given also by (2.1). We denote for short the set (d_0, d_2) as d . Let $|\phi(d)\rangle$ be an approximated ground state of the considered nucleus with a given deformation d . State $|\phi(d)\rangle$ is supposed to be the ground state of the mean-field Hamiltonian, either the phenomenological or the self-consistent one with constraints for the quadrupole moment. For all possible values of d states $|\phi(d)\rangle$ form a set of states called the intrinsic states in the following. The normalization of the intrinsic state is assumed to be:

$$\langle \phi(d) | \phi(d) \rangle = 1 \quad (2.2)$$

for every d .

In general, the state $|\phi(d)\rangle$ is not an irreducible representation of $O^T(3)$ because the rotational symmetry is usually broken spontaneously in the mean field. However, it is assumed that $|\phi(d)\rangle$ is still invariant under the point D_{2h}^T group [32] with the intrinsic axes (x, y, z) as its symmetry axes and we have:

$$\hat{T}|\phi(d)\rangle = |\phi(d)\rangle, \quad (2.3a)$$

$$e^{-i\pi\hat{J}_u}|\phi(d)\rangle = |\phi(d)\rangle, \quad (2.3b)$$

$$\hat{P}|\phi(d)\rangle = |\phi(d)\rangle, \quad (2.3c)$$

where \hat{J}_u for $u = x, y, z$ are the intrinsic components of the total angular momentum operator. Equation (2.3a) can be fulfilled only for even Z and N and, as a matter of fact, it corresponds to the assumption that we will consider only the even-even nuclei here. Although the D_{2h}^T symmetry looks natural, the parity invariance (2.3c) will not be used explicitly in further considerations. It is because the quadrupole deformation tensor itself is of the positive parity. Since the differentiation with respect to the deformation parameters d commutes with the D_{2h}^T generators the states

$$|\phi_k(d)\rangle = \frac{\partial}{\partial d_k}|\phi(d)\rangle, \quad |\phi_{kl}(d)\rangle = \frac{\partial^2}{\partial d_k \partial d_l}|\phi(d)\rangle, \quad \dots \quad (2.4)$$

for $k, l = 0, 2$ have also the D_{2h}^T symmetry and fulfil (2.3a), (2.3b) and (2.3c).

It follows from time reversal invariance that the matrix elements obey relations

$$\begin{aligned} \langle \phi(d) | \phi(d') \rangle &= \langle \phi(d) | \phi(d') \rangle^* = \langle \phi(d') | \phi(d) \rangle, \\ \langle \phi(d) | \hat{H} | \phi(d') \rangle &= \langle \phi(d) | \hat{H} | \phi(d') \rangle^* = \langle \phi(d') | \hat{H} | \phi(d) \rangle, \end{aligned} \quad (2.5)$$

i.e. they are real and symmetric with respect to d and d' . On the other hand, matrix elements $\langle \phi(d) | \hat{J}_u | \phi(d') \rangle$ and $\langle \phi(d) | \hat{J}_u \hat{H} | \phi(d') \rangle$ are imaginary and antisymmetric, because the angular momentum operators \hat{J}_u are time odd.

It follows from the D_2 symmetry (2.3b) of $|\phi(d)\rangle$ and $|\phi_i(d)\rangle$ that, in particular, the matrix elements of type $\langle\phi_i(d)|\hat{J}_u|\phi(d)\rangle$, $\langle\phi_i(d)|\hat{J}_u\hat{H}|\phi(d)\rangle$, and $\langle\phi(d)|\hat{J}_u\hat{J}_{u'}|\phi(d)\rangle$, $\langle\phi(d)|\hat{J}_u\hat{J}_{u'}\hat{H}|\phi(d)\rangle$ for $u \neq u'$ all vanish.

Since $|\phi(d)\rangle$ does not possess the rotational symmetry, the state rotated by the three Euler angles $\omega = (\omega_1, \omega_2, \omega_3)$ from the ranges $0 \leq \omega_1 < 2\pi$, $0 \leq \omega_2 \leq \pi$, $0 \leq \omega_3 < 2\pi$

$$|\Phi(d, \omega)\rangle = \hat{R}(\omega)|\phi(d)\rangle \quad (2.6)$$

is an equally good ground state of the mean-field Hamiltonian. The unitarity of $\hat{R}(\omega)$ assures us that it is also normalised to 1. Operator $\hat{R}(\omega)$ is time-even and thus the matrix elements between states $|\Phi(d, \omega)\rangle$ and $|\Phi(d', \omega')\rangle$ corresponding to these of (2.5) are also real and symmetric with respect to sets of variables (d, ω) and (d', ω') . States (2.6) will play the role of the generating states and the five variables $d_0, d_2, \omega_1, \omega_2$ and ω_3 can be used as the generator coordinates for the quadrupole collective excitations. As a matter of fact, other generator coordinates, namely the laboratory quadrupole deformations defined below will be used.

2.2. Quadrupole coordinates

We introduce a new set of the five variables, namely α_μ , $\mu = -2, \dots, +2$, by the relation

$$\alpha_\mu = d_0 D_{\mu 0}(\omega) + d_2 D_{\mu 2}(\omega), \quad (2.7)$$

where the semi-Cartesian Wigner functions $D_{\mu 0}$ and $D_{\mu 2}$, defined by (A.1), are combinations of the usual Wigner functions $\mathcal{D}_{\mu\nu}^2$. They play the role of the laboratory deformation parameters. The Jacobian of transformation (2.7) is equal to (cf [1])

$$W(d, \omega) = |d_2(3d_0^2 - d_2^2)| \sin \omega_2 \quad (2.8)$$

and, therefore, the transformation is reversible in the entire assumed open ranges of variables d and ω . It is seen from (2.7) that α_μ are the components of an electric (i.e. with positive parity), real (i.e. $\alpha_\mu^* = (-1)^\mu \alpha_{-\mu}$) quadrupole tensor $\boldsymbol{\alpha}$ in the three-dimensional physical space. The complex conjugate components are denoted with the superscript, e.g.

$$\alpha^\mu = \alpha_\mu^* = (-1)^\mu \alpha_{-\mu}. \quad (2.9)$$

The frame of axes with orientation $\omega = 0$ is the frame of principal axes (intrinsic frame) of $\boldsymbol{\alpha}$, because the intrinsic components of $\boldsymbol{\alpha}$ are equal to $\alpha_0(\omega = 0) = d_0$, $\alpha_2(\omega = 0) = \alpha_{-2}(\omega = 0) = d_2/\sqrt{2}$ and $\alpha_1(\omega = 0) = \alpha_{-1}(\omega = 0) = 0$.

Instead of the complex spherical components of the tensor, the five truly real coordinates a_k , $k = 0, 2, x, y, z$, namely

$$a_k = D_k^\mu(\omega = 0)\alpha_\mu = C_k^\mu \alpha_\mu \quad (2.10)$$

can be used, where the Einstein contraction rule is applied to summing of the Greek upper and lower indices $\mu = -2, \dots, +2$ of the spherical components. The rule is not applied to the Latin Cartesian indices. These coordinates can be treated as the

Cartesian components of vector \mathbf{a} in the five-dimensional space. This is because the scalar product of the two quadrupole tensors, $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ is

$$\boldsymbol{\alpha} \cdot \boldsymbol{\beta} = \sum_{\mu} (-1)^{\mu} \alpha_{\mu} \beta_{-\mu} = \alpha_{\mu} \beta^{\mu} = \sum_k a_k b_k = \mathbf{a} \cdot \mathbf{b}. \quad (2.11)$$

In connexion with (2.11) the volume element in the space of the quadrupole coordinates is:

$$d\Omega(\boldsymbol{\alpha}) = \Pi_k da_k = |d_2(3d_0^2 - d_2^2)| \sin \omega_2 dd_0 dd_2 d\omega_1 d\omega_2 d\omega_3. \quad (2.12)$$

All functions of deformation d and the Euler angles, ω , can be treated as functions of either tensor $\boldsymbol{\alpha}$ or vector \mathbf{a} . Here, we prefer to use the complex variables, α_{μ} , for convenience. However, we have in mind that the integration variables are always real: either a_k or d and ω as is seen in (2.12). The relation between the derivatives with respect to α_{μ} and the derivatives with respect to the Euler angles and the intrinsic components d_0, d_2 reads [41, 1]:

$$\begin{aligned} \frac{\partial}{\partial \alpha_{\mu}} &= \sum_k C_k^{\mu} \frac{\partial}{\partial a_k} \\ &= D_0^{\mu}(\omega) \frac{\partial}{\partial d_0} + D_2^{\mu}(\omega) \frac{\partial}{\partial d_2} + iD_z^{\mu}(\omega) \frac{1}{2d_z} L_z(\omega) \\ &\quad - iD_x^{\mu}(\omega) \frac{1}{2d_x} L_x(\omega) - iD_y^{\mu}(\omega) \frac{1}{2d_y} L_y(\omega), \end{aligned} \quad (2.13)$$

where

$$d_x = -\frac{1}{2}(\sqrt{3}d_0 + d_2), \quad d_y = \frac{1}{2}(\sqrt{3}d_0 - d_2), \quad d_z = d_2 \quad (2.14)$$

and $L_x(\omega)$, $L_y(\omega)$, $L_z(\omega)$ are differential operators with respect to the Euler angles and are interpreted as the intrinsic components of the drift angular momentum of the rotation of the intrinsic frame (eq. (2.15) in ref. [1]).

2.3. Trial states for the collective quadrupole excitations

We denote the generating states (2.6) as $|\Phi(\boldsymbol{\alpha})\rangle$. Then trial states for the quadrupole collective motion are taken in the form:

$$|\Psi[\varphi]\rangle = \int \varphi(\boldsymbol{\alpha}) |\Phi(\boldsymbol{\alpha})\rangle d\Omega(\boldsymbol{\alpha}). \quad (2.15)$$

The five components of the quadrupole tensor $\boldsymbol{\alpha}$ play the role of the generator coordinates and function $\varphi(\boldsymbol{\alpha})$ is the weight function. The variational principle leads to the Hill-Wheeler integral equation of the form

$$\int [\mathcal{H}(\boldsymbol{\alpha}, \boldsymbol{\alpha}') - E\mathcal{I}(\boldsymbol{\alpha}, \boldsymbol{\alpha}')] \varphi(\boldsymbol{\alpha}') d\Omega(\boldsymbol{\alpha}') = 0 \quad (2.16)$$

for function φ of the generator coordinates. The equation is determined by the two real symmetric kernels: the overlap kernel

$$\mathcal{I}(\boldsymbol{\alpha}, \boldsymbol{\alpha}') = \langle \Phi(\boldsymbol{\alpha}) | \Phi(\boldsymbol{\alpha}') \rangle \quad (2.17)$$

and the energy kernel

$$\mathcal{H}(\boldsymbol{\alpha}, \boldsymbol{\alpha}') = \langle \Phi(\boldsymbol{\alpha}) | \hat{H} | \Phi(\boldsymbol{\alpha}') \rangle. \quad (2.18)$$

The overlap kernel (2.17) is non-diagonal and equation (2.16) for the weight functions constitutes a non-orthogonal eigenvalue equation.

3. The Gaussian Overlap Approximation

3.1. Gaussian approximation for the kernels

We expect that the overlap kernel drops quickly from one to zero when differences $\gamma_\mu = \alpha_\mu - \alpha'_\mu$ of the components of tensors $\boldsymbol{\alpha}$ and $\boldsymbol{\alpha}'$ increase from zero. Therefore, the logarithm of the kernel rather than the kernel itself as a function of $\boldsymbol{\gamma}$ can be approximated by the power series:

$$\ln \mathcal{I}(\boldsymbol{\beta} + \tfrac{1}{2}\boldsymbol{\gamma}, \boldsymbol{\beta} - \tfrac{1}{2}\boldsymbol{\gamma}) = -\tfrac{1}{2}g^{\mu\nu}(\boldsymbol{\beta})\gamma_\mu\gamma_\nu + \dots, \quad (3.1)$$

where $\boldsymbol{\beta} = \tfrac{1}{2}(\boldsymbol{\alpha} + \boldsymbol{\alpha}')$ and the Einstein contraction rule is applied to upper and lower indices μ, ν . When in expansion (3.1) we keep only the term quadratic in $\boldsymbol{\gamma}$ for an arbitrary $\boldsymbol{\beta}$, we have the local Gaussian approximation for the overlap kernel:

$$\mathcal{I}(\boldsymbol{\beta} + \tfrac{1}{2}\boldsymbol{\gamma}, \boldsymbol{\beta} - \tfrac{1}{2}\boldsymbol{\gamma}) = \exp\left(-\tfrac{1}{2}g^{\mu\nu}(\boldsymbol{\beta})\gamma_\mu\gamma_\nu\right). \quad (3.2)$$

Matrix \mathbf{g} is real, symmetric and positive definite. We use a similar approximation for quotient

$$\frac{\mathcal{H}(\boldsymbol{\beta} + \tfrac{1}{2}\boldsymbol{\gamma}, \boldsymbol{\beta} - \tfrac{1}{2}\boldsymbol{\gamma})}{\mathcal{I}(\boldsymbol{\beta} + \tfrac{1}{2}\boldsymbol{\gamma}, \boldsymbol{\beta} - \tfrac{1}{2}\boldsymbol{\gamma})} = v(\boldsymbol{\beta}) - \tfrac{1}{2}h^{\mu\nu}(\boldsymbol{\beta})\gamma_\mu\gamma_\nu + \dots \quad (3.3)$$

Matrix \mathbf{h} is real and symmetric.

Both matrices, $g_{\mu\nu}$ and $h_{\mu\nu}$, are the symmetric quadrupole bitensors in the interpretation of Appendix B, whereas v a scalar. We shall refer to matrix \mathbf{g} as the metric tensor. Throughout the paper the upper and lower indices of matrices are connected with the complex conjugation of the spherical tensors according to (2.9), and not with the contravariant and covariant components of tensors in the Riemannian space. A separate symbol is used for the inverse metric tensor, namely $\mathbf{g}^{-1} = \mathbf{f}$.

3.2. Eigenvalue equation for the Gaussian overlap kernel

To find the eigenfunctions of the Gaussian overlap kernel (3.2) it is convenient to reduce the exponent of the Gaussian function to the sum of squares of five variables. It is a simple thing to do for the single generator coordinate [33]. It is not so simple in the case of a set of a few variables. Here, we adopt the definition of the new variables given by Onishi and Une [17]. Namely, we introduce the five new real variables t_k ($k=0, 2, x, y, z$) through a line integral in the five-dimensional space of vectors \mathbf{a} of (2.10)

$$t_k(\mathbf{a}) = \int^{\mathbf{a}} \sum_l r_{kl}(\mathbf{a}') d\mathbf{a}'_l. \quad (3.4)$$

The lower integration limit is omitted in the notation of the integral because it is not relevant here. Matrix \mathbf{r} is taken to be the positive-definite symmetric square root matrix of \mathbf{g} defined by (B.8) with $\mathbf{m} = \mathbf{g}$ and $\mathbf{m}^{1/2} = \mathbf{r}$. It fulfils relation (B.7), namely

$$g_{kl}(\mathbf{a}) = \sum_i r_{ki}(\mathbf{a})r_{il}(\mathbf{a}), \quad (3.5)$$

where g_{kl} are the Cartesian components of \mathbf{g} defined according to (B.4). The variables t_k are defined well if the line integral does not depend on the path of integration. It is so for the irrotational field $r_{kl}(\mathbf{a})$ i.e. for

$$\frac{\partial r_{kl}}{\partial a_i} - \frac{\partial r_{ki}}{\partial a_l} = 0, \quad (3.6)$$

which we assume for use of further considerations. However, we do not know in advance whether it is really fulfilled.

It is convenient to operate with the complex linear combinations τ_μ of t_k defined according to (2.10). Then we have

$$d\tau_\mu(\boldsymbol{\alpha}) = \sum_{k,l} C_{\mu k} C_l^\nu r_{kl}(\mathbf{a}) da_l = r_\mu^\nu(\boldsymbol{\alpha}) d\alpha_\nu, \quad (3.7)$$

where $r_\mu^\nu = r_\mu^\nu = r_\mu^\nu$ are the corresponding spherical components of \mathbf{r} (the sequence of the superscript and subscript does not need to be fixed for a symmetric matrix). Relations (3.5) and (3.6) have the following counterparts for the spherical components:

$$g_{\mu\nu}(\boldsymbol{\alpha}) - r_\mu^\lambda(\boldsymbol{\alpha})r_{\lambda\nu}(\boldsymbol{\alpha}) = \sum_{k,l} \left(C_{\mu k} C_{\nu l} \left(g_{kl}(\mathbf{a}) - \sum_i r_{ki}(\mathbf{a})r_{il}(\mathbf{a}) \right) \right) = 0, \quad (3.8)$$

$$\frac{\partial r_\mu^\nu}{\partial \alpha_\lambda} - \frac{\partial r_\mu^\lambda}{\partial \alpha_\nu} = \sum_{k,l,i} C_{\mu k} C_l^\nu C_i^\lambda \left(\frac{\partial r_{kl}}{\partial a_i} - \frac{\partial r_{ki}}{\partial a_l} \right) = 0. \quad (3.9)$$

The Jacobian of transformation $\boldsymbol{\tau} = \boldsymbol{\tau}(\boldsymbol{\alpha})$ is equal to $\sqrt{g(\boldsymbol{\alpha})} > 0$, where $g = \det(\mathbf{g})$. The transformation is then reversible. The reversed transformation is denoted as $\boldsymbol{\alpha} = \boldsymbol{\alpha}(\boldsymbol{\tau})$. The volume element in the space of $\boldsymbol{\tau}$ is

$$d\Omega(\boldsymbol{\tau}) = \sqrt{g(\boldsymbol{\alpha})} d\Omega(\boldsymbol{\alpha}). \quad (3.10)$$

When we assume that the values of $\gamma_\mu = \alpha_\mu - \alpha'_\mu$ are small, what is consistent with the Gaussian approximation, we have from (3.7):

$$\vartheta_\mu = \tau_\mu - \tau'_\mu = r_\mu^\nu \left(\frac{1}{2}(\boldsymbol{\alpha} + \boldsymbol{\alpha}') \right) (\alpha_\nu - \alpha'_\nu) = r_\mu^\nu(\boldsymbol{\beta}) \gamma_\nu, \quad (3.11a)$$

$$\theta_\mu = \frac{1}{2}(\tau_\mu + \tau'_\mu) = \tau_\mu(\boldsymbol{\beta}), \quad (3.11b)$$

where $\tau'_\mu = \tau_\mu(\boldsymbol{\alpha}')$.

Using the new variables, $\boldsymbol{\tau}$, it is easy to solve the eigenvalue equation

$$\int \mathcal{I}(\boldsymbol{\alpha}(\boldsymbol{\tau}), \boldsymbol{\alpha}(\boldsymbol{\tau}')) \chi(\boldsymbol{\epsilon}, \boldsymbol{\tau}') d\Omega(\boldsymbol{\tau}') = j(\boldsymbol{\epsilon}) \chi(\boldsymbol{\epsilon}, \boldsymbol{\tau}). \quad (3.12)$$

for the Gaussian overlap. The wave tensor $\boldsymbol{\epsilon}$ stands for a set of the five quantum numbers, ϵ_μ ($\mu = -2, \dots, 2$), which label eigenfunctions $\chi(\boldsymbol{\epsilon}, \boldsymbol{\tau})$ and eigenvalues $j(\boldsymbol{\epsilon})$. The normalised eigenfunction reads:

$$\chi(\boldsymbol{\epsilon}, \boldsymbol{\tau}) = \frac{1}{(2\pi)^{5/2}} \exp(i\boldsymbol{\epsilon} \cdot \boldsymbol{\tau}). \quad (3.13)$$

It fulfils the following orthogonality and completeness conditions:

$$\int \chi^*(\epsilon, \tau) \chi(\epsilon', \tau) d\Omega(\tau) = \delta_5(\epsilon - \epsilon'), \quad (3.14a)$$

$$\int \chi^*(\epsilon, \tau) \chi(\epsilon, \tau') d\Omega(\epsilon) = \delta_5(\tau - \tau'). \quad (3.14b)$$

The tensor properties of quantum numbers ϵ_μ are clearly seen from (3.13). The eigenvalue is equal to:

$$j(\epsilon) = (2\pi)^{5/2} \exp(-\frac{1}{2}\epsilon \cdot \epsilon). \quad (3.15)$$

3.3. The orthogonal Hill-Wheeler equation in GOA

We know that the Hill-Wheeler equation (2.16) can be formally reduced to the orthogonal eigenvalue equation (cf [12]) for wave-function $\psi(\alpha)$ defined as follows:

$$\psi(\alpha) = \int \mathcal{R}(\alpha, \alpha') \varphi(\alpha') d\Omega(\alpha'), \quad (3.16)$$

where

$$\mathcal{R}(\alpha, \xi) = \int \chi(\epsilon, \tau(\alpha)) j^{1/2}(\epsilon) \chi^*(\epsilon, \tau(\xi)) d\Omega(\epsilon) \quad (3.17)$$

is the square root kernel. The name of \mathcal{R} is justified by the relation

$$\int \mathcal{R}(\alpha, \xi) \mathcal{R}(\xi, \alpha') d\Omega(\tau(\xi)) = \mathcal{I}(\alpha, \alpha'). \quad (3.18)$$

Equation (3.16) can be formally reversed and the weight function, φ can be expressed in the form:

$$\varphi(\alpha) = \int \mathcal{N}(\alpha, \xi) \psi(\xi) d\Omega(\tau(\xi)), \quad (3.19)$$

where the narrowing kernel [11]

$$\mathcal{N}(\alpha, \xi) = \int \chi(\epsilon, \tau(\alpha)) j^{-1/2}(\epsilon) \chi^*(\epsilon, \tau(\xi)) d\Omega(\epsilon) \quad (3.20)$$

is introduced, which fulfils the following relation:

$$\int \mathcal{R}(\alpha, \xi) \mathcal{N}(\xi, \alpha') d\Omega(\tau(\xi)) = \delta_5(\tau(\alpha) - \tau(\alpha')). \quad (3.21)$$

We define the narrowed overlap kernel

$$\begin{aligned} \mathcal{J}(\xi, \xi') &= \int \mathcal{N}^*(\alpha, \xi) \mathcal{I}(\alpha(\tau), \alpha'(\tau)) \mathcal{N}(\alpha', \xi') d\Omega(\tau(\alpha)) d\Omega(\tau(\alpha')) \\ &= \delta_5(\tau(\xi) - \tau(\xi')), \end{aligned} \quad (3.22)$$

which takes the diagonal form.

To obtain the integral eigenvalue equation for function ψ we substitute (3.19) for the weight function, φ in the Hill-Wheeler equation (2.16), multiply it by $\mathcal{N}(\alpha, \xi)$ and integrate with respect to $\tau(\alpha)$. Then we get

$$\int \mathcal{K}(\xi, \xi') \psi(\xi') d\Omega(\tau(\xi')) = E \psi(\xi), \quad (3.23)$$

where

$$\mathcal{K}(\xi, \xi') = \int \mathcal{N}^*(\alpha, \xi) \mathcal{H}(\alpha, \alpha') \mathcal{N}(\alpha', \xi') d\Omega(\tau(\alpha)) d\Omega(\tau(\alpha')) \quad (3.24)$$

is the narrowed energy kernel.

3.4. The Fourier analysis of the Gaussian energy kernel

The problem with equation (3.23), and kernels (3.20) and (3.24) is that eigenvalues $j(\epsilon)$ of the Gaussian overlap kernel tend to zero when $\epsilon \cdot \epsilon$ tends to infinity. It means that the integral in (3.20) is divergent and we have the "ultra-violet catastrophe" for \mathcal{N} . To make the integral convergent we can introduce a cut-off for $\epsilon \cdot \epsilon$. Instead, we can use operational methods of the distribution theory and treat integrals being the Fourier transforms of the non-integrable functions as convergent due to oscillations with the infinite frequencies of the integrand and express them by the Dirac delta function and its derivatives, namely

$$\frac{1}{2\pi} \int_{-\infty}^{+\infty} f(k) e^{ikx} dk = f(-i d/dx) \delta(x). \quad (3.25)$$

Equation (3.25) follows from the formula for the derivatives of the delta function represented in the form of the Fourier integral, namely:

$$\left(-i \frac{d}{dx}\right)^n \delta(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} k^n e^{ikx} dk \quad (3.26)$$

for $n = 0, 1, \dots$

In order to express the Gaussian energy kernel in terms of the delta function and its derivatives we introduce the Fourier transform, \mathcal{F} , of \mathcal{H} in the following way:

$$\mathcal{F}(\epsilon, \epsilon') = \int \chi^*(\epsilon, \tau(\alpha)) \mathcal{H}(\alpha, \alpha') \chi(\epsilon', \tau(\alpha')) d\Omega(\tau(\alpha)) d\Omega(\tau(\alpha')). \quad (3.27)$$

Substituting (3.3), (3.11a), (3.11b) and (3.13) into (3.27) we have

$$\begin{aligned} \mathcal{F}(\epsilon, \epsilon') &= \frac{1}{(2\pi)^5} \int [v(\beta) - \frac{1}{2} a^{\kappa\lambda}(\beta) \vartheta_\kappa(\beta, \gamma) \vartheta_\lambda(\beta, \gamma)] \\ &\times \exp(-i\sigma \cdot \theta(\beta)) \exp(-\frac{1}{2} \vartheta(\beta, \gamma) \cdot \vartheta(\beta, \gamma) - i\epsilon \cdot \vartheta(\beta, \gamma)) d\Omega(\theta(\beta)) d\Omega(\vartheta(\beta, \gamma)), \end{aligned} \quad (3.28)$$

where

$$a_{\kappa\lambda}(\beta) = h^{\mu\nu}(\beta) n_{\mu\kappa}(\beta) n_{\lambda\nu}(\beta) \quad (3.29)$$

and $\epsilon = \frac{1}{2}(\epsilon + \epsilon')$, $\sigma = \epsilon - \epsilon'$, and $n_{\mu\nu} = (1/\sqrt{g})(\partial\sqrt{g}/\partial r^{\mu\nu})$ is the matrix reversed to r , i.e. $n_{\nu\lambda} r^{\lambda\mu} = \delta_\nu^\mu$. The Gaussian integrals with respect to ϑ can be easily calculated and we obtain

$$\mathcal{F}(\epsilon, \epsilon') = \frac{j(\epsilon)}{(2\pi)^5} \int [v(\beta) + \frac{1}{2}(\epsilon^\kappa \epsilon_\lambda - \delta_\lambda^\kappa) a_\kappa^\lambda(\beta)] \exp(-i\sigma \cdot \theta(\beta)) d\Omega(\theta(\beta)). \quad (3.30)$$

The narrowed energy kernel (3.24) expressed in terms of the Fourier transform (3.27) reads:

$$\mathcal{K}(\xi, \xi') = \int j^{-1/2}(\epsilon) j^{-1/2}(\epsilon') \chi(\epsilon, \xi) \mathcal{F}(\epsilon, \epsilon') \chi^*(\epsilon', \xi') d\Omega(\epsilon) d\Omega(\epsilon'). \quad (3.31)$$

Inserting (3.13), (3.15) and (3.30) into (3.31) we have

$$\begin{aligned} \mathcal{K}(\boldsymbol{\xi}, \boldsymbol{\xi}') &= \frac{1}{(2\pi)^{10}} \int \exp\left(\frac{1}{8}\boldsymbol{\sigma} \cdot \boldsymbol{\sigma}\right) \exp\left(\mathbf{i}\boldsymbol{\sigma} \cdot (\boldsymbol{\theta}(\boldsymbol{\eta}) - \boldsymbol{\theta}(\boldsymbol{\beta}))\right) d\Omega(\boldsymbol{\sigma}) \\ &\times [v(\boldsymbol{\beta}) + \frac{1}{2}(\varepsilon^\kappa \varepsilon_\lambda - \delta_\lambda^\kappa) a_\kappa^\lambda(\boldsymbol{\beta})] \exp(\mathbf{i}\boldsymbol{\varepsilon} \cdot \boldsymbol{\vartheta}(\boldsymbol{\eta}, \boldsymbol{\zeta})) d\Omega(\boldsymbol{\varepsilon}) d\Omega(\boldsymbol{\theta}(\boldsymbol{\beta})), \end{aligned} \quad (3.32)$$

where $\boldsymbol{\eta} = \frac{1}{2}(\boldsymbol{\xi} + \boldsymbol{\xi}')$ and $\boldsymbol{\zeta} = \boldsymbol{\xi} - \boldsymbol{\xi}'$. The integrals with respect to $\boldsymbol{\varepsilon}$ and $\boldsymbol{\sigma}$ in (3.32) are the fivefold integrals of type (3.25) and thus can be expressed in terms of the partial derivatives of the five-dimensional Dirac δ function in the following way:

$$\begin{aligned} &\frac{1}{(2\pi)^5} \int [v(\boldsymbol{\beta}) + \frac{1}{2}(\varepsilon^\kappa \varepsilon_\lambda - \delta_\lambda^\kappa) a_\kappa^\lambda(\boldsymbol{\beta})] \exp(\mathbf{i}\boldsymbol{\varepsilon} \cdot \boldsymbol{\vartheta}(\boldsymbol{\eta}, \boldsymbol{\zeta})) d\Omega(\boldsymbol{\varepsilon}) \\ &= \left[v(\boldsymbol{\beta}) + \frac{1}{2} \left(\left(-\mathbf{i} \frac{\partial}{\partial \vartheta_\kappa(\boldsymbol{\eta}, \boldsymbol{\zeta})} \right) \left(-\mathbf{i} \frac{\partial}{\partial \vartheta^\lambda(\boldsymbol{\eta}, \boldsymbol{\zeta})} \right) - \delta_\lambda^\kappa \right) a_\kappa^\lambda(\boldsymbol{\beta}) \right] \delta_5(\boldsymbol{\vartheta}(\boldsymbol{\eta}, \boldsymbol{\zeta})), \end{aligned} \quad (3.33)$$

$$\begin{aligned} &\frac{1}{(2\pi)^5} \int \exp\left(\frac{1}{8}\boldsymbol{\sigma} \cdot \boldsymbol{\sigma}\right) \exp\left(\mathbf{i}\boldsymbol{\sigma} \cdot (\boldsymbol{\theta}(\boldsymbol{\eta}) - \boldsymbol{\theta}(\boldsymbol{\beta}))\right) d\Omega(\boldsymbol{\sigma}) \\ &= \exp\left(\frac{1}{8} \left(-\mathbf{i} \frac{\partial}{\partial \theta_\mu(\boldsymbol{\eta})} \right) \left(-\mathbf{i} \frac{\partial}{\partial \theta^\mu(\boldsymbol{\eta})} \right) \right) \delta_5(\boldsymbol{\theta}(\boldsymbol{\eta}) - \boldsymbol{\theta}(\boldsymbol{\beta})). \end{aligned} \quad (3.34)$$

After inserting (3.33) and (3.34) into (3.32) the integration with respect to $\boldsymbol{\theta}(\boldsymbol{\beta})$ is easily performed and finally the narrowed energy kernel takes the form:

$$\begin{aligned} \mathcal{K}(\boldsymbol{\xi}, \boldsymbol{\xi}') &= \exp\left(-\frac{1}{8}\Delta(\boldsymbol{\theta}(\boldsymbol{\eta}))\right) \\ &\times \left[v(\boldsymbol{\eta}) - \frac{1}{2}h^{\mu\nu}(\boldsymbol{\eta})f_{\mu\nu}(\boldsymbol{\eta}) - \frac{1}{2}a_\kappa^\lambda(\boldsymbol{\eta}) \frac{\partial}{\partial \vartheta^\kappa(\boldsymbol{\eta}, \boldsymbol{\zeta})} \frac{\partial}{\partial \vartheta^\lambda(\boldsymbol{\eta}, \boldsymbol{\zeta})} \right] \delta_5(\boldsymbol{\vartheta}(\boldsymbol{\eta}, \boldsymbol{\zeta})), \end{aligned} \quad (3.35)$$

where $\mathbf{f} = \mathbf{g}^{-1} = \mathbf{n} \cdot \mathbf{n}$ is the matrix reversed to \mathbf{g} , and

$$\Delta(\boldsymbol{\tau}) = \frac{\partial}{\partial \tau_\mu} \frac{\partial}{\partial \tau^\mu}. \quad (3.36)$$

The kernel is thus the distribution dependent on the delta function of $\boldsymbol{\vartheta}(\boldsymbol{\xi}, \boldsymbol{\xi}') = \boldsymbol{\tau}(\boldsymbol{\xi}) - \boldsymbol{\tau}(\boldsymbol{\xi}')$ and its partial derivatives of the second order. We rewrite it in a shorter form:

$$\mathcal{K}(\boldsymbol{\xi}, \boldsymbol{\xi}') = \left[\bar{v}'(\boldsymbol{\eta}) - \frac{1}{2}\bar{a}_\kappa^\lambda(\boldsymbol{\eta}) \frac{\partial}{\partial \vartheta^\kappa(\boldsymbol{\eta}, \boldsymbol{\zeta})} \frac{\partial}{\partial \vartheta^\lambda(\boldsymbol{\eta}, \boldsymbol{\zeta})} \right] \delta_5(\boldsymbol{\vartheta}(\boldsymbol{\eta}, \boldsymbol{\zeta})), \quad (3.37)$$

where

$$\bar{a}_{\mu\nu}(\boldsymbol{\eta}) = \exp\left(-\frac{1}{8}\Delta(\boldsymbol{\theta}(\boldsymbol{\eta}))\right) a_{\mu\nu}(\boldsymbol{\eta}), \quad (3.38a)$$

$$\bar{v}'(\boldsymbol{\eta}) = \exp\left(-\frac{1}{8}\Delta(\boldsymbol{\theta}(\boldsymbol{\eta}))\right) \left[v(\boldsymbol{\eta}) - \frac{1}{2}h^{\mu\nu}(\boldsymbol{\eta})f_{\mu\nu}(\boldsymbol{\eta}) \right] = \exp\left(-\frac{1}{8}\Delta(\boldsymbol{\theta}(\boldsymbol{\eta}))\right) v'(\boldsymbol{\eta}). \quad (3.38b)$$

4. Differential eigenvalue equations

4.1. The differential Hill-Wheeler equation

The integral Hill-Wheeler equation (3.23) is easily converted into a differential equation using the kernel in the form of (3.35). Indeed, inserting (3.35) into (3.23) we have:

$$\begin{aligned} &\int \psi(\boldsymbol{\xi}') \left[\bar{v}'\left(\frac{1}{2}(\boldsymbol{\xi} + \boldsymbol{\xi}')\right) - \frac{1}{2}\bar{a}_\kappa^\lambda\left(\frac{1}{2}(\boldsymbol{\xi} + \boldsymbol{\xi}')\right) \frac{\partial}{\partial \tau^\kappa(\boldsymbol{\xi}')} \frac{\partial}{\partial \tau^\lambda(\boldsymbol{\xi}')}\right] \delta_5(\boldsymbol{\tau}(\boldsymbol{\xi}) - \boldsymbol{\tau}(\boldsymbol{\xi}')) d\Omega(\boldsymbol{\tau}(\boldsymbol{\xi}')) \\ &= E\psi(\boldsymbol{\xi}). \end{aligned} \quad (4.1)$$

Integrating by parts we obtain from (4.1) the following differential eigenvalue equation:

$$\left[-\frac{1}{2} \frac{\partial}{\partial \tau_\mu(\boldsymbol{\xi})} \bar{a}_{\mu\nu}(\boldsymbol{\xi}) \frac{\partial}{\partial \tau_\nu(\boldsymbol{\xi})} + \bar{V}(\boldsymbol{\xi}(\boldsymbol{\tau})) \right] \psi(\boldsymbol{\xi}) = E \psi(\boldsymbol{\xi}), \quad (4.2)$$

where

$$\bar{V}(\boldsymbol{\xi}) = \bar{v}'(\boldsymbol{\xi}) - \frac{1}{8} \frac{\partial^2 \bar{a}_{\mu\nu}(\boldsymbol{\xi})}{\partial \tau_\mu(\boldsymbol{\xi}) \partial \tau_\nu(\boldsymbol{\xi})}. \quad (4.3)$$

Coming back to the original variables $\boldsymbol{\xi}$ in (4.2) we transform the derivatives with respect to $\tau_\mu(\boldsymbol{\xi})$ into the derivatives with respect to ξ_μ and we obtain the eigenvalue equation

$$\bar{H}(\boldsymbol{\xi}) \psi(\boldsymbol{\xi}) = E \psi(\boldsymbol{\xi}) \quad (4.4)$$

for the Bohr Hamiltonian

$$\bar{H}(\boldsymbol{\xi}) = -\frac{1}{2\sqrt{g(\boldsymbol{\xi})}} \frac{\partial}{\partial \xi_\mu} \sqrt{g(\boldsymbol{\xi})} \bar{A}_{\mu\nu}(\boldsymbol{\xi}) \frac{\partial}{\partial \xi_\nu} + \bar{V}(\boldsymbol{\xi}) \quad (4.5)$$

with the inverse inertial bitensor

$$\bar{A}_{\mu\nu}(\boldsymbol{\xi}) = n_{\mu\kappa}(\boldsymbol{\xi}) n_{\nu\lambda}(\boldsymbol{\xi}) \bar{a}^{\kappa\lambda}(\boldsymbol{\xi}) \quad (4.6)$$

and the potential

$$\bar{V}(\boldsymbol{\xi}) = \exp\left(-\frac{1}{8}\Delta(\boldsymbol{\xi})\right) v'(\boldsymbol{\xi}) - \frac{1}{8} \frac{1}{\sqrt{g(\boldsymbol{\xi})}} \frac{\partial}{\partial \xi_\mu} \left(\sqrt{g(\boldsymbol{\xi})} n_{\mu\kappa}(\boldsymbol{\xi}) n_{\nu\lambda}(\boldsymbol{\xi}) \frac{\partial \bar{a}^{\kappa\lambda}(\boldsymbol{\xi})}{\partial \xi_\nu} \right). \quad (4.7)$$

The Laplacian (3.36) takes the form:

$$\Delta(\boldsymbol{\xi}) = \frac{1}{\sqrt{g(\boldsymbol{\xi})}} \frac{\partial}{\partial \xi_\mu} \sqrt{g(\boldsymbol{\xi})} f_{\mu\nu}(\boldsymbol{\xi}) \frac{\partial}{\partial \xi_\nu}. \quad (4.8)$$

The relation

$$\frac{\partial}{\partial \xi_\mu} \left(\sqrt{g(\boldsymbol{\xi})} n_{\mu\nu}(\boldsymbol{\xi}) \right) = 0, \quad (4.9)$$

which comes from (3.6), has been used to obtain (4.5), (4.7) and (4.8).

Equation (4.4) is equivalent to the Hill-Wheeler equation (3.23) with the Gaussian plus quadratic approximation (3.2) and (3.3) for the kernels. No other approximation is made. However, one can say that the equivalence is formal only because the quantities (4.6) and (4.7) can be determined merely in an approximation when expanding the exponential operator. For instance, we expand (3.38a):

$$\bar{a}_{\mu\nu}(\boldsymbol{\xi}) = a_{\mu\nu}(\boldsymbol{\xi}) - \frac{1}{8} \Delta(\boldsymbol{\xi}) a_{\mu\nu}(\boldsymbol{\xi}) + \frac{1}{2} \left(\frac{1}{8} \right)^2 \Delta(\boldsymbol{\xi}) \Delta(\boldsymbol{\xi}) a_{\mu\nu}(\boldsymbol{\xi}) + \dots \quad (4.10)$$

However, we have no guarantee whether such an approximation procedure is convergent.

4.2. The collective Hamiltonian

Another method of deriving the Bohr Hamiltonian, which passes by the integral equation (3.23) and starts directly from the variational principle, is more often used (cf [12, 19, 20]). We refer to it as the collective approach to the GCM. It consists in representing the energy mean value in the form of the expectation value of a local differential operator, say H , Hermitian with weight w in the space of the generator coordinates, namely:

$$\begin{aligned}\langle \Psi[\varphi] | \hat{H} | \Psi[\varphi] \rangle &= \int \varphi^*(\alpha) \mathcal{H}(\alpha, \alpha') \varphi(\alpha') d\Omega(\alpha) d\Omega(\alpha') \\ &= \int \psi^*(\alpha) H(\alpha) \psi(\alpha) w(\alpha) d\Omega(\alpha).\end{aligned}\quad (4.11)$$

In the GOA the square root kernel (3.17) is equal to

$$\mathcal{R}(\alpha, \xi) = \left(\frac{2}{\pi}\right)^{5/4} \exp(-(\tau(\alpha) - \tau(\xi)) \cdot (\tau(\alpha) - \tau(\xi))) \quad (4.12)$$

and then, according to (3.18) and (3.3) the energy kernel can be presented in the following form

$$\begin{aligned}\mathcal{H}(\alpha, \alpha') &= \int \mathcal{R}(\alpha, \xi) [v(\beta) - \frac{1}{2} h^{\mu\nu}(\beta) \gamma_\mu \gamma_\nu] \mathcal{R}(\xi, \alpha') \sqrt{g(\xi)} d\Omega(\xi) \\ &= \int \mathcal{R}(\alpha, \xi) [v(\beta) - \frac{1}{2} a^{\mu\nu}(\beta) \vartheta_\mu(\alpha, \alpha') \vartheta_\nu(\alpha, \alpha')] \mathcal{R}(\xi, \alpha') d\Omega(\tau(\xi)).\end{aligned}\quad (4.13)$$

An additional approximation should be made to achieve the form (4.11) for the energy functional. Namely, we assume that functions $v(\beta)$ and $a^{\mu\nu}(\beta)$ do not change much within the range of $\beta = \frac{1}{2}(\alpha + \alpha')$ in the vicinity of ξ where both Gaussian functions, $\mathcal{R}(\alpha, \xi)$ and $\mathcal{R}(\xi, \alpha')$ take still big values. In other words we assume that $v(\beta)$ and $a^{\mu\nu}(\beta)$ are slowly varying functions in the vicinity of ξ , and we can expand them in the power series around ξ :

$$v(\beta) \approx v(\xi) + \frac{\partial v(\xi)}{\partial \xi_\mu} (\beta_\mu - \xi_\mu) + \frac{1}{2} \frac{\partial^2 v(\xi)}{\partial \xi_\mu \partial \xi_\nu} (\beta_\mu - \xi_\mu) (\beta_\nu - \xi_\nu) + \dots \quad (4.14a)$$

$$a^{\mu\nu}(\beta) \approx a^{\mu\nu}(\xi) + \frac{\partial a^{\mu\nu}(\xi)}{\partial \xi_\kappa} (\beta_\kappa - \xi_\kappa) + \frac{1}{2} \frac{\partial^2 a^{\mu\nu}(\xi)}{\partial \xi_\kappa \partial \xi_\lambda} (\beta_\kappa - \xi_\kappa) (\beta_\lambda - \xi_\lambda) + \dots \quad (4.14b)$$

in (4.13). Here, we will exploit the lowest approximation and take the zero-order terms only. Since the Gaussian functions with monomial factors in front are equal to the derivatives of the Gaussian functions themselves, the α - and α' -dependence of the integrand in (4.13) appear only in functions $\mathcal{R}(\alpha, \xi)$ and $\mathcal{R}(\xi, \alpha')$ and their derivatives with respect to ξ_μ . Then, the integration with respect α and α' in (4.11) can be performed giving the collective wave-functions $\psi^*(\xi)$ and $\psi(\xi)$ of (3.16). Finally, we can obtain the energy mean value in the form (4.11) performing integrations by parts. The collective Hamiltonian in the space of coordinates $\tau(\xi)$ reads

$$H = -\frac{1}{2} \frac{\partial}{\partial \tau_\mu(\xi)} a_{\mu\nu}(\xi) \frac{\partial}{\partial \tau_\nu(\xi)} + V(\xi) \quad (4.15)$$

with $a_{\mu\nu}$ given by (3.29) and

$$\begin{aligned} V(\boldsymbol{\xi}) &= v(\boldsymbol{\xi}) - \frac{1}{2}h^{\mu\nu}(\boldsymbol{\xi})f_{\mu\nu}(\boldsymbol{\xi}) - \frac{1}{8}\frac{\partial^2 a_{\mu\nu}(\boldsymbol{\xi})}{\partial\tau_\mu(\boldsymbol{\xi})\partial\tau_\nu(\boldsymbol{\xi})} \\ &= v'(\boldsymbol{\xi}) - \frac{1}{8}\frac{\partial^2 a_{\mu\nu}(\boldsymbol{\xi})}{\partial\tau_\mu(\boldsymbol{\xi})\partial\tau_\nu(\boldsymbol{\xi})}. \end{aligned} \quad (4.16)$$

Coming back to variables $\boldsymbol{\xi}$ we end up with the collective Bohr Hamiltonian

$$H = -\frac{1}{2\sqrt{g(\boldsymbol{\xi})}}\frac{\partial}{\partial\xi_\mu}\sqrt{g(\boldsymbol{\xi})}A_{\mu\nu}(\boldsymbol{\xi})\frac{\partial}{\partial\xi_\nu} + V(\boldsymbol{\xi}), \quad (4.17)$$

Hermitian with weight $w(\boldsymbol{\xi}) = \sqrt{g(\boldsymbol{\xi})}$, where

$$A_{\mu\nu}(\boldsymbol{\xi}) = f_{\mu\kappa}(\boldsymbol{\xi})f_{\nu\lambda}(\boldsymbol{\xi})h^{\kappa\lambda}(\boldsymbol{\xi}) \quad (4.18)$$

and

$$\begin{aligned} V(\boldsymbol{\xi}) &= v(\boldsymbol{\xi}) - \frac{1}{2}h^{\mu\nu}(\boldsymbol{\xi})f_{\mu\nu}(\boldsymbol{\xi}) \\ &\quad - \frac{1}{8}\frac{1}{\sqrt{g(\boldsymbol{\xi})}}\frac{\partial}{\partial\xi_\mu}\left(\sqrt{g(\boldsymbol{\xi})}n_{\mu\kappa}(\boldsymbol{\xi})n_{\nu\lambda}(\boldsymbol{\xi})\frac{\partial a^{\kappa\lambda}(\boldsymbol{\xi})}{\partial\xi_\nu}\right). \end{aligned} \quad (4.19)$$

We see that the Bohr Hamiltonians \bar{H} and H have the same form which is identical with that discussed in [1] for the quantum collective models. The only difference between them is that they are determined by different inverse inertial bitensors and different collective potentials, $\bar{A}_{\mu\nu}$ and $A_{\mu\nu}$, and \bar{V} and V , respectively. For $\exp(-\frac{1}{8}\Delta) \approx 1$ the quantities with bar transform into the corresponding quantities without bar. Such an approximation is good when $a_{\mu\nu}(\boldsymbol{\xi})$ and $v(\boldsymbol{\xi})$ are slowly varying functions of their argument. It is in accordance with the assumption made when deriving Hamiltonian H of (4.17).

4.3. The zero-point energy

In the original approach to the Bohr Hamiltonian, there is an ambiguity related to the correspondence principle. The Podolsky-Pauli quantization prescription tells us how to quantize the kinetic energy; however, in general, the kinetic energy operator is given up to an additive arbitrary function of the deformation [8]. In consequence, the potential energy which enters the Bohr Hamiltonian operator needs not to be identical with the classical one, as has been often assumed in the past (cf [1]). In the present study it would correspond to the collective potential $V(d) = v(d) = \langle\phi(d)|\hat{H}|\phi(d)\rangle$ equal to the static ground-state energy term. On the other hand, it is obvious that dynamical correlations in the ground state of quantum systems should appear. Various effects of the ground-state correlations have been investigated for a long time (see, e.g., a review [34]). In the theory of the collective excitations, the difference between the static energy and the collective potential is interpreted as the zero-point energy associated with a given collective mode. The GCM gives a definite result for the zero-point energy correction to the static ground-state energy. The zero-point energies associated with the quadrupole vibrational modes have been already estimated in the frame of the GOA,

e.g., [36, 35, 21, 22, 37]. Those associated with the rotational modes were investigated rather by means of the angular-momentum projection technique [22, 37].

In the present five-dimensional GCM with the set of generator coordinates forming the quadrupole tensor, all the quadrupole modes, both vibrational and rotational are treated on an equal footing. The collective potential of (4.19) contains the zero-point energy correction, $v(\boldsymbol{\xi}) - V(\boldsymbol{\xi})$, associated with all the five quadrupole modes. We see from (4.19) that the correction is composed of two terms. The first, $\frac{1}{2}\mathbf{f} \cdot \mathbf{h}$, is connected with the quadratic term in the energy kernel expansion (3.3) and manifests the dynamical effects. The second one appears only when the coefficients in the Gaussian expansions (3.2) and (3.3), $g_{\mu\nu}(\boldsymbol{\beta})$ and $h_{\mu\nu}(\boldsymbol{\beta})$, depend essentially on $\boldsymbol{\beta}$ (the case of the local Gaussian approximation). The additional zero-point energy corrections come from expanding the exponential Laplace operator in (3.38a) and (3.38b) as discussed in section 4.1. Then, additional terms appear in both, the inverse inertial bitensor, $\bar{A}_{\mu\nu}$, and the potential, \bar{V} , in the Bohr Hamiltonian \bar{H} of (4.5). It seems that corrections of that type to the zero-point energy have been taken into account in [21] for the one-dimensional Bohr Hamiltonian. In our case of the five-dimensional quadrupole modes a counterpart of the collective potential with similar corrections would have perhaps the form:

$$\bar{V}(\boldsymbol{\xi}) = (1 - \frac{1}{8}\Delta(\boldsymbol{\xi}))v'(\boldsymbol{\xi}) - \frac{1}{8} \frac{1}{\sqrt{g(\boldsymbol{\xi})}} \frac{\partial}{\partial \xi_\mu} \left(\sqrt{g(\boldsymbol{\xi})} n_{\mu\kappa}(\boldsymbol{\xi}) n_{\nu\lambda}(\boldsymbol{\xi}) \frac{\partial a^{\kappa\lambda}(\boldsymbol{\xi})}{\partial \xi_\nu} \right). \quad (4.20)$$

The standard procedure of deriving the collective Hamiltonian, shown in [12, 19, 20], consists in expanding quotient $\mathcal{H}(\boldsymbol{\alpha}, \boldsymbol{\alpha}')/\mathcal{I}(\boldsymbol{\alpha}, \boldsymbol{\alpha}')$ of (3.3) (the expression inside the square brackets in (4.13)) as a function of $\boldsymbol{\alpha}$ and $\boldsymbol{\alpha}'$ in the power series around an arbitrary point $\boldsymbol{\xi}$ up to the second order. The actual meaning of the approximation is not very transparent. Certainly, it constitutes a stronger approximation than the usual quadratic approximation of (3.3) in the GOA. It seems that a counterpart of such an approximation in the present approach is expanding the static potential (4.14a) up to the second order. Then, the resulting collective potential would have the form:

$$\begin{aligned} \bar{V}(\boldsymbol{\xi}) = & (1 - \frac{1}{8}\Delta(\boldsymbol{\xi}))v(\boldsymbol{\xi}) - \frac{1}{2}h^{\mu\nu}(\boldsymbol{\xi})f_{\mu\nu}(\boldsymbol{\xi}) \\ & - \frac{1}{8} \frac{1}{\sqrt{g(\boldsymbol{\xi})}} \frac{\partial}{\partial \xi_\mu} \left(\sqrt{g(\boldsymbol{\xi})} n_{\mu\kappa}(\boldsymbol{\xi}) n_{\nu\lambda}(\boldsymbol{\xi}) \frac{\partial a^{\kappa\lambda}(\boldsymbol{\xi})}{\partial \xi_\nu} \right). \end{aligned} \quad (4.21)$$

4.4. Matrix elements of observables

Solving the Bohr equation (4.4) (or that with Hamiltonian (4.17)) provides us with the energies, E_N , and the collective wave-functions, ψ_N , of the collective states

$$|\Psi_N\rangle = \int \mathcal{N}(\boldsymbol{\alpha}, \boldsymbol{\xi}) \psi_N(\boldsymbol{\xi}) |\Phi(\boldsymbol{\alpha})\rangle \sqrt{g(\boldsymbol{\xi})} d\Omega(\boldsymbol{\xi}) \sqrt{g(\boldsymbol{\alpha})} d\Omega(\boldsymbol{\alpha}), \quad (4.22)$$

where N stands for a set of quantum numbers of the state. The states form an orthonormal set, i.e., $\langle \Psi_N | \Psi_{N'} \rangle = \delta_{NN'}$ when

$$\int \psi_N^*(\boldsymbol{\xi}) \psi_{N'}(\boldsymbol{\xi}) \sqrt{g(\boldsymbol{\xi})} d\Omega(\boldsymbol{\xi}) = \delta_{NN'}. \quad (4.23)$$

To know other characteristics of the collective states we should calculate the matrix elements of the other observables. In the GOA we approximate the matrix element of observable \hat{Q} within states $|\Phi(\alpha)\rangle$ in the way similar to (3.3):

$$\langle \Phi(\alpha) | \hat{Q} | \Phi(\alpha') \rangle = q(\beta) + iq^\mu(\beta)\gamma_\mu - \frac{1}{2}q^{\mu\nu}(\beta)\gamma_\mu\gamma_\nu + \dots \quad (4.24)$$

Proceeding further in the way similar to that of sections 3.4 and 4.1 for \hat{H} we obtain

$$\begin{aligned} \langle \Psi_N | \hat{Q} | \Psi_{N'} \rangle = & \int \psi_N^*(\xi) \left[-\frac{1}{2} \frac{\partial}{\partial \xi_\mu} \sqrt{g(\xi)} \bar{Q}_{\mu\nu}(\xi) \frac{\partial}{\partial \xi_\nu} \right. \\ & - \frac{i}{2} \left(\frac{\partial}{\partial \xi_\mu} \sqrt{g(\xi)} \bar{Q}_\mu(\xi) + \sqrt{g(\xi)} \bar{Q}_\mu(\xi) \frac{\partial}{\partial \xi_\mu} \right) \\ & \left. + \sqrt{g(\xi)} \bar{Q}(\xi) \right] \psi_{N'}(\xi) d\Omega(\xi), \end{aligned} \quad (4.25)$$

where $\bar{Q}_{\mu\nu}$ and \bar{Q} are given by (4.6) and (4.7) when $h^{\alpha\beta}$ and v are replaced with $q^{\alpha\beta}$ and q , respectively, whereas

$$\bar{Q}_\mu(\xi) = n_{\mu\kappa}(\xi) \exp(-\frac{1}{8}\Delta(\xi)) [q^\alpha(\xi) n_\alpha^\kappa(\xi)], \quad (4.26)$$

and ψ_N are eigenfunctions of Hamiltonian \bar{H} .

When q , $n_\mu^\nu q_\nu$ and $n_\mu^\kappa q_{\kappa\lambda} n_\nu^\lambda$ are slowly varying functions of ξ the exponential Laplacian operator can be replaced by the unity and we have the expression similar in form with (4.25)(cf [25]), namely:

$$\begin{aligned} \langle \Psi_N | \hat{Q} | \Psi_{N'} \rangle = & \int \psi_N^*(\xi) \left[-\frac{1}{2} \frac{\partial}{\partial \xi_\mu} \sqrt{g(\xi)} Q_{\mu\nu}(\xi) \frac{\partial}{\partial \xi_\nu} \right. \\ & - \frac{i}{2} \left(\frac{\partial}{\partial \xi_\mu} \sqrt{g(\xi)} Q_\mu(\xi) + \sqrt{g(\xi)} Q_\mu(\xi) \frac{\partial}{\partial \xi_\mu} \right) \\ & \left. + \sqrt{g(\xi)} Q(\xi) \right] \psi_{N'}(\xi) d\Omega(\xi), \end{aligned} \quad (4.27)$$

where $Q_{\mu\nu}$, Q_μ and Q are given by the corresponding formulae for $\bar{Q}_{\mu\nu}$, \bar{Q}_μ and \bar{Q} with the exponential operator put equal to unity, and ψ_N are this time eigenfunctions of Hamiltonian H .

5. The deformation dependence of the quadrupole collective Hamiltonian

The original object in the present approach to the description of the quadrupole collective states in even-even nuclei is a set of the many-body intrinsic states $|\phi(d)\rangle$ parametrised by the two quadrupole deformations $d = (d_0, d_2)$. Knowing $|\phi(d)\rangle$ we can express the overlap and energy kernels, the two basic quantities in the Hill-Wheeler equation, in terms of overlaps and matrix elements of \hat{H} and \hat{J}_u within states $|\phi(d)\rangle$ themselves and their derivatives (2.4). All these overlaps and matrix elements are functions of the deformation. Having the kernels as functions of the deformation we calculate the collective potential and inertial functions which determine the Bohr Hamiltonian.

5.1. The overlap and energy kernels as functions of deformation

The overlap kernel $\mathcal{I}(\boldsymbol{\alpha}, \boldsymbol{\alpha}')$ is real, symmetric and normalised to unity for the all values of variables α_μ , namely

$$\mathcal{I}(\boldsymbol{\alpha}, \boldsymbol{\alpha}) = \langle \Phi(\boldsymbol{\alpha}) | \Phi(\boldsymbol{\alpha}) \rangle = 1. \quad (5.1a)$$

Differentiating twice (5.1a) we have the following conditions:

$$\langle \Phi(\boldsymbol{\alpha}) | \Phi^\mu(\boldsymbol{\alpha}) \rangle = 0, \quad (5.1b)$$

$$\langle \Phi(\boldsymbol{\alpha}) | \Phi^{\mu\nu}(\boldsymbol{\alpha}) \rangle + \langle \Phi^\mu(\boldsymbol{\alpha}) | \Phi^\nu(\boldsymbol{\alpha}) \rangle = 0, \quad (5.1c)$$

where

$$|\Phi^\mu(\boldsymbol{\alpha})\rangle = \frac{\partial}{\partial \alpha_\mu} |\Phi(\boldsymbol{\alpha})\rangle, \quad |\Phi^{\mu\nu}(\boldsymbol{\alpha})\rangle = \frac{\partial^2}{\partial \alpha_\mu \partial \alpha_\nu} |\Phi(\boldsymbol{\alpha})\rangle \quad (5.2)$$

are the states created by differentiation with respect to the components of tensor $\boldsymbol{\alpha}$.

The GOA consists technically in expanding the logarithm of overlap kernel in powers of $\boldsymbol{\gamma} = \boldsymbol{\alpha} - \boldsymbol{\alpha}'$ up to the second order in $\boldsymbol{\gamma}$. The coefficients of expansion are the partial derivatives of $\ln \mathcal{I}(\boldsymbol{\beta} + \frac{1}{2}\boldsymbol{\gamma}, \boldsymbol{\beta} - \frac{1}{2}\boldsymbol{\gamma})$ at $\boldsymbol{\gamma} = 0$. They are:

$$\begin{aligned} \left. \frac{\partial \ln \mathcal{I}(\boldsymbol{\beta} + \frac{1}{2}\boldsymbol{\gamma}, \boldsymbol{\beta} - \frac{1}{2}\boldsymbol{\gamma})}{\partial \gamma_\mu} \right|_{\gamma_{-2}=\dots=\gamma_2=0} &\equiv \frac{\partial \ln \mathcal{I}(\boldsymbol{\beta}, \boldsymbol{\beta})}{\partial \gamma_\mu} \\ &= \frac{\langle \Phi^\mu(\boldsymbol{\beta}) | \Phi(\boldsymbol{\beta}) \rangle - \langle \Phi(\boldsymbol{\beta}) | \Phi^\mu(\boldsymbol{\beta}) \rangle}{2\langle \Phi(\boldsymbol{\beta}) | \Phi(\boldsymbol{\beta}) \rangle} = 0 \end{aligned} \quad (5.3a)$$

in virtue of (5.1a) and (5.1b), and in accordance with (3.1).

$$\begin{aligned} \frac{\partial^2 \ln \mathcal{I}(\boldsymbol{\beta}, \boldsymbol{\beta})}{\partial \gamma_\mu \partial \gamma_\nu} &= -(\mathcal{I}(\boldsymbol{\beta}, \boldsymbol{\beta}))^{-2} \frac{\partial \mathcal{I}(\boldsymbol{\beta}, \boldsymbol{\beta})}{\partial \gamma_\mu} \frac{\partial \mathcal{I}(\boldsymbol{\beta}, \boldsymbol{\beta})}{\partial \gamma_\nu} + (\mathcal{I}(\boldsymbol{\beta}, \boldsymbol{\beta}))^{-1} \frac{\partial^2 \mathcal{I}(\boldsymbol{\beta}, \boldsymbol{\beta})}{\partial \gamma_\mu \partial \gamma_\nu} \\ &= \frac{\partial^2 \mathcal{I}(\boldsymbol{\beta}, \boldsymbol{\beta})}{\partial \gamma_\mu \partial \gamma_\nu} \end{aligned} \quad (5.3b)$$

according to (5.1a) and (5.3a). Hence, the metric tensor defined by (3.1) is

$$g^{\mu\nu}(\boldsymbol{\beta}) = -\frac{\partial^2 \mathcal{I}(\boldsymbol{\beta}, \boldsymbol{\beta})}{\partial \gamma_\mu \partial \gamma_\nu}. \quad (5.4)$$

Performing the second order derivative and using additionally (5.1c) we have finally

$$g^{\mu\nu}(\boldsymbol{\alpha}) = \langle \Phi^\mu(\boldsymbol{\alpha}) | \Phi^\nu(\boldsymbol{\alpha}) \rangle. \quad (5.5)$$

State $|\Phi(\boldsymbol{\alpha})\rangle$ is of the form of (2.6). Thus, using (2.13) we replace the derivatives with respect to α_μ in (5.5) by the derivatives with respect to the Euler angles ω and deformations d . The ω -dependence of $|\Phi(\boldsymbol{\alpha})\rangle$ is inherent in $\hat{R}(\omega)$. Differentiating the rotation operator with respect to the Euler angles we obtain the formula

$$L_u(\omega) \hat{R}(\omega) = -\hat{R}(\omega) \hat{J}_u \quad \text{for } u = x, y, z. \quad (5.6)$$

Finally, $g^{\mu\nu}(\boldsymbol{\alpha})$ is obtained in the following form (cf (B.1)):

$$g^{\mu\nu}(\boldsymbol{\alpha}) = \sum_{a,b} D_a^\mu(\omega) D_b^\nu(\omega) g_{ab}(d), \quad (5.7)$$

where $a, b = 0, 2, x, y, z$. The intrinsic Cartesian components are:

$$g_{kl}(d) = \langle \phi_k(d) | \phi_l(d) \rangle \quad \text{for } k, l = 0, 2, \quad (5.8a)$$

$$g_{uu}(d) = \frac{1}{4d_u^2} \langle \phi(d) | \hat{J}_u^2 | \phi(d) \rangle \quad \text{for } u = x, y, z \quad (5.8b)$$

$$g_{ku}(d) = g_{uu'}(d) = 0 \quad \text{for } k = 0, 2, u, u' = x, y, z, u \neq u', \quad (5.8c)$$

where $|\phi_k(d)\rangle$ are given by (2.4) and d_u is defined in (2.14). The intrinsic Cartesian components of (5.8c) vanish owing to the assumed symmetries of $|\phi(d)\rangle$ discussed in section 2.3. The weight appearing in the Bohr Hamiltonian of (4.17) is, according to (B.3), equal to

$$\sqrt{g(d)} = \sqrt{(g_{00}(d)g_{22}(d) - g_{02}^2(d))g_{xx}(d)g_{yy}(d)g_{zz}(d)}. \quad (5.9)$$

The intrinsic Cartesian components of matrix \mathbf{f} inverse to \mathbf{g} and its square root matrix \mathbf{n} which appear in (4.18) and (4.19) can be calculated from (5.8a) and (5.8b) according to (B.8) and (B.6).

In the Gaussian approximation the energy kernel $\mathcal{H}(\boldsymbol{\alpha}, \boldsymbol{\alpha}')$ is given by (3.3). The zero order term in the expansion is

$$v(\boldsymbol{\alpha}) = v(d) = \frac{\mathcal{H}(\boldsymbol{\alpha}, \boldsymbol{\alpha})}{\mathcal{I}(\boldsymbol{\alpha}, \boldsymbol{\alpha})} = \langle \phi(d) | \hat{H} | \phi(d) \rangle. \quad (5.10)$$

The second order term is defined by the matrix of the second order partial derivatives of quotient \mathcal{H}/\mathcal{I} at $\boldsymbol{\gamma} = 0$ as follows:

$$h^{\mu\nu}(\boldsymbol{\beta}) = -\frac{\partial^2}{\partial\gamma_\mu\partial\gamma_\nu} \left(\frac{\mathcal{H}(\boldsymbol{\beta}, \boldsymbol{\beta})}{\mathcal{I}(\boldsymbol{\beta}, \boldsymbol{\beta})} \right), \quad (5.11)$$

where the notation of (5.3a) is used. Due to (5.1a), (5.3a) and (5.4) we have:

$$\begin{aligned} h^{\mu\nu}(\boldsymbol{\beta}) &= -\frac{\partial^2 \mathcal{H}(\boldsymbol{\beta}, \boldsymbol{\beta})}{\partial\gamma_\mu\partial\gamma_\nu} + \frac{\partial^2 \mathcal{I}(\boldsymbol{\beta}, \boldsymbol{\beta})}{\partial\gamma_\mu\partial\gamma_\nu} \mathcal{H}(\boldsymbol{\beta}, \boldsymbol{\beta}) \\ &= -\frac{\partial^2 \mathcal{H}(\boldsymbol{\beta}, \boldsymbol{\beta})}{\partial\gamma_\mu\partial\gamma_\nu} - g^{\mu\nu}(\boldsymbol{\beta})v(\boldsymbol{\beta}). \end{aligned} \quad (5.12)$$

After replacing the derivatives with respect to γ_μ by the derivatives with respect to α_μ \mathbf{h} takes the following form

$$\begin{aligned} h^{\mu\nu}(\boldsymbol{\alpha}) &= \frac{1}{2} \left[\langle \Phi^\mu(\boldsymbol{\alpha}) | \hat{H} | \Phi^\nu(\boldsymbol{\alpha}) \rangle - \langle \Phi(\boldsymbol{\alpha}) | \hat{H} | \Phi^{\mu\nu}(\boldsymbol{\alpha}) \rangle \right] \\ &\quad - \langle \Phi^\mu(\boldsymbol{\alpha}) | \Phi^\nu(\boldsymbol{\alpha}) \rangle \langle \Phi(\boldsymbol{\alpha}) | \hat{H} | \Phi(\boldsymbol{\alpha}) \rangle. \end{aligned} \quad (5.13)$$

Differentiation with respect to α_μ by means of (2.13) gives naturally \mathbf{h} in the form of (B.1) with the following intrinsic Cartesian components which do not vanish:

$$h_{kl}(d) = \frac{1}{2} [\langle \phi_k(d) | \hat{H} | \phi_l(d) \rangle - \langle \phi(d) | \hat{H} | \phi_{kl}(d) \rangle] - \langle \phi_k(d) | \phi_l(d) \rangle \langle \phi(d) | \hat{H} | \phi(d) \rangle \quad (5.14a)$$

for $k, l = 0, 2,$

$$h_{uu}(d) = \frac{1}{4d_u^2} \left[\langle \phi(d) | \hat{H} \hat{J}_u^2 | \phi(d) \rangle - \langle \phi(d) | \hat{J}_u^2 | \phi(d) \rangle \langle \phi(d) | \hat{H} | \phi(d) \rangle \right] \quad (5.14b)$$

for $u = x, y, z.$

The remaining intrinsic components vanish for the symmetry reasons (cf section 2.3).

We see that in order to calculate v , \mathbf{g} and \mathbf{h} , and then the inverse inertial bitensor and the collective potential we should calculate the mean values of the squares of angular momenta \hat{J}_u^2 , Hamiltonian \hat{H} and their products $\hat{J}_u^2 \hat{H}$ within the deformation dependent intrinsic ground state $|\phi(d)\rangle$, construct the states $|\phi_k(d)\rangle$ and $|\phi_{kl}(d)\rangle$ through differentiations of $|\phi(d)\rangle$ with respect to the deformation parameters d and calculate their overlaps and matrix elements of \hat{H} within them.

5.2. Inverse inertial functions and potential

The intrinsic Cartesian components of the inverse inertial bitensor (4.18) do not depend on the Euler angles ω and are functions of deformation d only. We refer to the corresponding intrinsic components $A_{ab}(d)$, ($a, b = 0, 2, x, y, z$) of matrix $A_{\mu\nu}(\boldsymbol{\alpha})$ as the inverse inertial functions. It results from (4.18) using (A.3), (B.1) and (B.6) that the inverse inertial vibrational functions are equal to

$$A_{00}(d) = \frac{g_{22}^2(d)h_{00}(d) - 2g_{02}(d)g_{22}(d)h_{02}(d) + g_{02}^2(d)h_{22}(d)}{(g_{00}(d)g_{22}(d) - g_{02}^2(d))^2}, \quad (5.15a)$$

$$A_{02}(d) = \frac{(g_{00}(d)g_{22}(d) + g_{02}^2(d))h_{02}(d) - g_{02}(d)g_{22}(d)h_{00}(d) - g_{02}g_{00}(d)h_{22}(d)}{(g_{00}(d)g_{22}(d) - g_{02}^2(d))^2}, \quad (5.15b)$$

$$A_{22}(d) = \frac{g_{02}^2(d)h_{00}(d) - 2g_{02}(d)g_{00}(d)h_{02}(d) + g_{22}^2(d)h_{22}(d)}{(g_{00}(d)g_{22}(d) - g_{02}^2(d))^2} \quad (5.15c)$$

and the inverse inertial rotational functions read

$$A_{uu}(d) = \frac{h_{uu}(d)}{g_{uu}^2(d)} \quad (5.15d)$$

for $u = x, y, z$. Hence, the moments of inertia by definition (cf [1]) are

$$I_u(d) = \frac{4d_u^2}{A_{uu}(d)} = \frac{\langle \phi(d) | \hat{J}_u^2 | \phi(d) \rangle^2}{\langle \phi(d) | \hat{H} \hat{J}_u^2 | \phi(d) \rangle - \langle \phi(d) | \hat{J}_u^2 | \phi(d) \rangle \langle \phi(d) | \hat{H} | \phi(d) \rangle}. \quad (5.16)$$

They resemble the Yoccoz moment of inertia [38, 39] and are in form similar to those of a rigid body [31].

Being a quadrupole scalar, the collective potential depends obviously on deformation d only. Equation (4.19) for the potential contains matrices \mathbf{n} and \mathbf{a} . Their intrinsic Cartesian components can be calculated from (B.6), (B.8) and (3.29). It is worth noting that the zero-point energy corrections associated with the rotational modes come not only from the rotational components (of type a_{uu} , $u = x, y, z$) of the matrices involved in the corresponding formula for the potential and the derivatives of these matrices with respect to d but also from the derivatives with respect to ω coming from the differentiation of (2.13) with respect to α_μ . These latter derivatives can be performed using (B.1) and (A.5). Obviously, the final result for the potential does not depend on the Euler angles.

6. Conclusions

Using the GCM we have generated the quadrupole collective excitations from the deformation-dependent intrinsic ground state which possesses the D_{2h}^T symmetry. To consider not only the quadrupole vibrations but also the quadrupole rotations the intrinsic state is rotated and the three Euler angles of the rotation are attached to the two deformation parameters and form together the real electric quadrupole tensor which plays a role of a set of generator coordinates. It turns out convenient to use just the quadrupole tensor, the real components of which are the Cartesian coordinates in the five-dimensional space, instead of the Euler angles and the deformation parameters. In this way, periodic coordinates and a complicated topology of the space are avoided. The local GOA has been applied to the overlap and energy kernels. In this case the integral Hill-Wheeler equation can be reduced to the differential equation having the form of the eigenvalue equation for the Bohr Hamiltonian. The reduction has been performed using the Fourier analysis of the energy kernel. The square root of determinant of the matrix defining the overlap in the GOA (the metric tensor) is the weight in the Bohr Hamiltonian. The exact potential and the inverse inertial bitensor contains the exponential function of the five-dimensional Laplacian operator and therefore, can be calculated only in an approximation. The simplest approximation consists in replacing the exponential operator by the first term of its expansion — the unit operator. This approximation corresponds to the potential and the inverse inertial bitensor obtained by the usual collective approach to the GCM. The next terms of the expansion can be, of course, taken into account in our approach, however, without settling the issue of convergence of the procedure.

When deriving the Bohr Hamiltonian, a transformation of the quadrupole variables must be performed, which transforms the metric tensor into the unit matrix. The resulting new set of variables is defined well when the square root matrix of the metric tensor is an irrotational field (cf [17]). Obviously, this condition is equivalent to the condition which means that the Riemannian space with the metric tensor in question being the Euclidean space. The assumption about the flatness of the space is apparently made in other papers on the multi-dimensional GOA even if this is not mentioned there (cf [18, 19]). The final form of the Bohr Hamiltonian does not seem to depend on this assumption. From the brief report by Kamlah [16] it seems that the assumption is not necessary, however, the proof of this fact has not been given there. Is it thus a technical condition coming from the fact that we are not able to calculate multi-dimensional Gaussian integrals? Or is it an essential condition? A similar problem appears in a sense in the case of the Podolsky-Pauli quantization prescription. The form of the quantum operator is simply assumed. However, if one would want to derive this form from the Schrödinger operator in the Euclidean space, one should assume that the new variables are curvilinear variables also in the Euclidean space and the kinetic energy is simply proportional to the Laplacian in curvilinear coordinates. It would then mean that the classical inertial matrix represents the metric tensor of an Euclidean space. We

are left with this open problem.

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Appendix A. Semi-Cartesian Wigner functions

The quadrupole tensors transform themselves under rotations by means of the rotation matrices or the Wigner functions $\mathcal{D}_{\mu\nu}^2(\omega)$ which depend on a set of the Euler angles defining the rotation [40]. It is convenient to introduce the following linear combinations of the Wigner functions [41]:

$$\begin{aligned} D_{\mu 0}(\omega) &= \mathcal{D}_{\mu 0}^2(\omega), \\ D_{\mu 2}(\omega) &= \frac{1}{\sqrt{2}}(\mathcal{D}_{\mu 2}^2(\omega) + \mathcal{D}_{\mu -2}^2(\omega)), \\ D_{\mu x}(\omega) &= \frac{i}{\sqrt{2}}(\mathcal{D}_{\mu 1}^2(\omega) + \mathcal{D}_{\mu -1}^2(\omega)), \\ D_{\mu y}(\omega) &= \frac{1}{\sqrt{2}}(\mathcal{D}_{\mu 1}^2(\omega) - \mathcal{D}_{\mu -1}^2(\omega)), \\ D_{\mu z}(\omega) &= \frac{i}{\sqrt{2}}(\mathcal{D}_{\mu 2}^2(\omega) - \mathcal{D}_{\mu -2}^2(\omega)). \end{aligned} \tag{A.1}$$

Let us call them the "semi-Cartesian" Wigner functions. The complex conjugate functions are

$$D_k^\mu(\omega) = D_{\mu k}^*(\omega) = (-1)^\mu D_{-\mu k}(\omega). \tag{A.2}$$

The orthogonality conditions for the semi-Cartesian Wigner functions take the form:

$$\sum_{\mu=-2}^2 D_k^\mu(\omega) D_{\mu l}(\omega) = \delta_{kl}, \tag{A.3}$$

$$\sum_k D_k^\mu(\omega) D_{\nu k}(\omega) = \delta_\nu^\mu. \tag{A.4}$$

The drift angular momentum operators $L_u(\omega)$, $u = x, y, z$, act on the semi-Cartesian Wigner functions as follows [41]

$$\begin{aligned} L_x(\omega) D_{\mu 0}(\omega) &= -i\sqrt{3} D_{\mu x}(\omega), \quad L_x(\omega) D_{\mu y}(\omega) = -i D_{\mu z}(\omega), \\ L_x(\omega) D_{\mu x}(\omega) &= i\sqrt{3} D_{\mu 0}(\omega) + i D_{\mu 2}(\omega), \\ L_x(\omega) D_{\mu z}(\omega) &= i D_{\mu y}(\omega), \quad L_x(\omega) D_{\mu 2}(\omega) = -i D_{\mu x}(\omega), \\ L_y(\omega) D_{\mu 0}(\omega) &= i\sqrt{3} D_{\mu y}(\omega), \quad L_y(\omega) D_{\mu x}(\omega) = i D_{\mu z}(\omega), \\ L_y(\omega) D_{\mu y}(\omega) &= -i\sqrt{3} D_{\mu 0}(\omega) + i D_{\mu 2}(\omega), \\ L_y(\omega) D_{\mu z}(\omega) &= -i D_{\mu x}(\omega), \quad L_y(\omega) D_{\mu 2}(\omega) = -i D_{\mu y}(\omega), \end{aligned} \tag{A.5}$$

$$\begin{aligned}
L_z(\omega)D_{\mu 0}(\omega) &= 0, \\
L_z(\omega)D_{\mu x}(\omega) &= iD_{\mu y}(\omega), \quad L_z(\omega)D_{\mu y}(\omega) = -iD_{\mu x}(\omega), \\
L_z(\omega)D_{\mu z}(\omega) &= 2iD_{\mu 2}(\omega), \quad L_z(\omega)D_{\mu 2}(\omega) = -2iD_{\mu z}(\omega).
\end{aligned}$$

It is seen that all the three components of the drift angular momentum change the Cartesian indices of the Wigner functions.

Appendix B. Symmetric matrices as isotropic functions of the quadrupole tensor

Any symmetric quadrupole bitensor (symmetric matrix 5×5) $m_{\mu\nu}(\alpha)$ which is an isotropic real function of the quadrupole tensor α can be determined either by six scalar functions of $d = (d_0, d_2)$ or by the six intrinsic Cartesian components in the following way (cf [1]):

$$m_{\mu\nu}(\alpha) = \sum_{k,l} D_{\mu k}(\omega) D_{\nu l}(\omega) m_{kl}(d), \quad (\text{B.1})$$

where the Cartesian indices k, l run over symbols 0, 2, x, y, z . The Euler angles ω determine the orientation of the intrinsic system. The Cartesian matrix $m_{kl}(d)$ is real symmetric and has the following structure:

$$\mathbf{m}(d) = \begin{pmatrix} m_{00}(d) & m_{02}(d) & 0 & 0 & 0 \\ m_{02}(d) & m_{22}(d) & 0 & 0 & 0 \\ 0 & 0 & m_{xx}(d) & 0 & 0 \\ 0 & 0 & 0 & m_{yy}(d) & 0 \\ 0 & 0 & 0 & 0 & m_{zz}(d) \end{pmatrix}. \quad (\text{B.2})$$

The determinant of \mathbf{m} reads

$$m = \det(\mathbf{m}) = (m_{00}m_{22} - m_{02}^2)m_{xx}m_{yy}m_{zz} = m_v^2 m_{xx}m_{yy}m_{zz}. \quad (\text{B.3})$$

The Cartesian components of matrix $\mathbf{m}(\alpha)$ are:

$$m_{kl}(\alpha) = C_k^\mu C_l^\nu m_{\mu\nu}(\alpha), \quad (\text{B.4})$$

where $C_k^\mu = D_k^\mu(\omega = 0)$.

If matrix $m_{\mu\nu}$ is not singular i.e. $m \neq 0$ matrix $(\mathbf{m}^{-1})_{\mu\nu}$ inverse to $m_{\mu\nu}$ can be defined as

$$m_{\mu\kappa}(\alpha)(\mathbf{m}^{-1})^{\kappa\nu}(\alpha) = \delta_\mu^\nu. \quad (\text{B.5})$$

The intrinsic Cartesian matrix inverse to \mathbf{m} is:

$$\begin{aligned}
&\mathbf{m}^{-1}(d) \\
&= \begin{pmatrix} m_{22}(d)/m_v^2(d) & -m_{02}(d)/m_v^2(d) & 0 & 0 & 0 \\ -m_{02}(d)/m_v^2(d) & m_{00}(d)/m_v^2(d) & 0 & 0 & 0 \\ 0 & 0 & 1/m_{xx}(d) & 0 & 0 \\ 0 & 0 & 0 & 1/m_{yy}(d) & 0 \\ 0 & 0 & 0 & 0 & 1/m_{zz}(d) \end{pmatrix}. \quad (\text{B.6})
\end{aligned}$$

If \mathbf{m} is positive definite i.e. m_{00} , m_{22} , m_{xx} , m_{yy} , m_{zz} and $m_v^2 = m_{00}m_{22} - m_{02}^2$ are all positive the positive-definite square root matrix $(\mathbf{m}^{1/2})_{\mu\nu}$ such that

$$m_v^\mu(\boldsymbol{\alpha}) = (\mathbf{m}^{1/2})_\kappa^\mu(\boldsymbol{\alpha})(\mathbf{m}^{1/2})_\nu^\kappa(\boldsymbol{\alpha}) \quad (\text{B.7})$$

can be defined. It is real symmetric and has the structure of (B.1) like \mathbf{m} . The nonvanishing entries of the intrinsic Cartesian matrix $(\mathbf{m}^{1/2})_{kl}$ are related to components m_{kl} as follows:

$$\begin{aligned} (\mathbf{m}^{1/2})_{00} &= \frac{m_{00} + m_v}{\sqrt{m_{00} + m_{22} + 2m_v}}, \\ (\mathbf{m}^{1/2})_{22} &= \frac{m_{22} + m_v}{\sqrt{m_{00} + m_{22} + 2m_v}}, \\ (\mathbf{m}^{1/2})_{02} &= \frac{m_{02}}{\sqrt{m_{00} + m_{22} + 2m_v}}, \\ (\mathbf{m}^{1/2})_{xx} &= \sqrt{m_{xx}}, \quad (\mathbf{m}^{1/2})_{yy} = \sqrt{m_{yy}}, \quad (\mathbf{m}^{1/2})_{zz} = \sqrt{m_{zz}}. \end{aligned} \quad (\text{B.8})$$

References

- [1] Próchniak L and Rohoziński S G 2009 *J. Phys. G: Nucl. Part. Phys.* **36** 123101
- [2] Bohr A 1952 *K. Danske Vidensk. Selsk., Mat.-Fys. Medd.* **26** No 14
- [3] Flügge S 1941 *Ann. Phys., Lpz.* **431** 373
- [4] Belyaev S T 1965 *Nucl. Phys.* **64** 17
- [5] Kumar K and Baranger M 1967 *Nucl. Phys. A* **92** 608
- [6] Podolsky B 1928 *Phys. Rev.* **32** 812
- [7] Pauli W 1980 *General Principles of Quantum Mechanics* (Berlin: Springer) p 94
- [8] Hofmann H 1972 *Z. Phys.* **250** 14
- [9] Baranger M, Kumar K 1968 *Nucl. Phys. A* **122** 241
- [10] Hill D L and Wheeler J A 1953 *Phys. Rev.* **89** 1102
- [11] Griffin J J and Wheeler J A 1957 *Phys. Rev.* **108** 311
- [12] Ring P and Schuck P 1980 *The Nuclear Many-Body Problem* (New York: Springer) Chapt 10
- [13] Haff P K and Wilets L 1973 *Phys. Rev. C* **7** 951
- [14] Jancovici B and Schiff D H 1964 *Nucl. Phys.* **58** 678
- [15] Brink D M and Weiguny A 1968 *Nucl. Phys. A* **120** 59
- [16] Kamlah A 1973 *Proc. Int. Conf. on Nuclear Physics (Munich)* vol 1 (Amsterdam: North Holland) p 127
- [17] Onishi N and Une T 1975 *Progr. Theor. Phys* **53** 504
- [18] Gózdź A 1985 *Phys. Lett.* **152B** 281
- [19] Gózdź A, Pomorski K, Brack M and Werner E 1985 *Nucl. Phys. A* **442** 26
- [20] Reinhard P-G and Goeke K 1987 *Rep. Prog. Phys.* **50** 1
- [21] Bonche P, Dobaczewski J, Flocard H, Heenen P-H and Meyer J 1990 *Nucl. Phys.* **A510** 466
- [22] Bonche P, Dobaczewski J, Flocard H and Heenen P-H 1991 *Nucl. Phys.* **A530** 149
- [23] Heenen P-H, Bonche P, Dobaczewski J and Flocard H 1993 *Nucl. Phys.* **A561** 367
- [24] Reinhard P-G 1978 *Z. Phys.* **285** A 93
- [25] Nerlo-Pomorska B, Pomorski K, Brack M and Werner E 1986 *Nucl. Phys.* **A462** 252
- [26] Staszczak A, Piłat S and Pomorski K 1989 *Nucl. Phys.* **A504** 589
- [27] Piłat S and Pomorski K 1993 *Nucl. Phys.* **A554** 413
- [28] Hagino K, Reinhard P-G and Bertsch G F 2002 *Phys. Rev. C* **65** 064320
- [29] Bertsch G F, Girod M, Hilaire S, Delaroche J-P, Goutte H and Péru S 2007 *Phys. Rev. Lett.* **99** 032502
- [30] Thouless D J and Valatin J G 1962 *Nucl. Phys.* **31** 211

- [31] Une T, Ikeda A and Onishi N 1976 *Prog. Theor. Phys.* **55** 498
- [32] Dobaczewski J, Dudek J, Rohoziński S G and Werner T R 2000 *Phys. Rev. C* **62** 014310
- [33] Ferreira L S and Caldeira M H 1971 *Nucl. Phys.* **A189** 250
- [34] Reinhard P-G and Toepffer C 1994 *Int. J. Mod. Phys. E* **3** 435
- [35] Girod M and Grammaticos B 1979 *Nucl. Phys.* **A330** 40
- [36] Reinhard P-G 1975 *Nucl. Phys.* **A252** 120
- [37] Hagino K, Bertsch G F and Reinhard P-G 2003 *Phys. Rev. C* **68** 024306
- [38] Peierls R E and Yoccoz J 1957 *Proc. Phys. Soc. (London)* **A70** 381
- [39] Yoccoz J 1957 *Proc. Phys. Soc. (London)* **A70** 388
- [40] Bohr A and Mottelson B R 1969 *Nuclear Structure* vol 1 (New York/Amsterdam: Benjamin) appendix 1A
- [41] Rohoziński S G, Gajda M and Greiner W 1982 *J. Phys. G: Nucl. Phys.* **8** 787